lsopropylpropyzamide 80045-52-9 | DTXSID40230046

Model Performance	

Model	Data

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 1.47e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.53e-01

Confidence level: 6.61e-01

Nearest Neighbors from the Training Set

Image not found

Thiophanate-methyl Measured: 4.35e-07 Predicted: 5.84e-08

Image not found

alpha-Fenchone Measured: 9.11e-04 Predicted: 5.32e-01

Image not found

2,2-Dimethylbutanoic acid Measured: 5.94e-05 Predicted: 1.90e-01

Image not found

2'-Acetonaphthone Measured: 6.63e-06 Predicted: 5.75e-04